Mitglied der Helmholtz-Gemeinschaft

JÜLICH
FORSCHUNGSZENTRUM

HPC Activities at Jülich Supercomputing Centre

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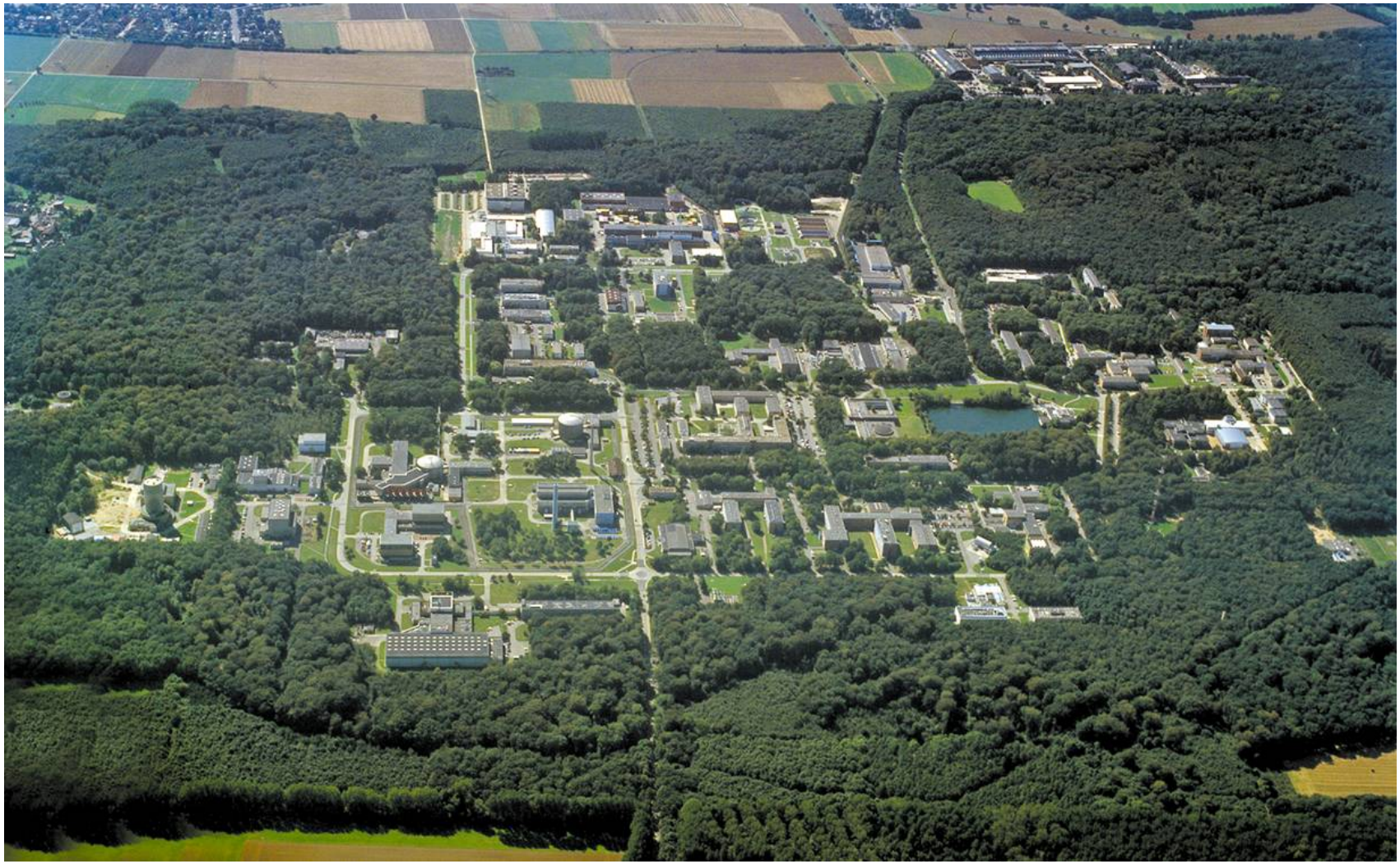
Jülich Supercomputing Centre

11th Workshop of the INRIA-Illinois-ANL
Joint Laboratory for PetaScale Computing
INRIA, Sophia Antipolis, 9. -11. June 2014

Forschungszentrum Jülich (FZJ)



Jülich Supercomputing Centre (JSC)

JÜLICH
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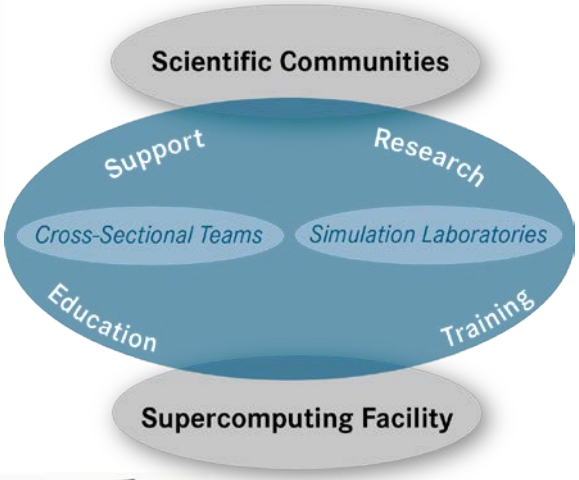
Jülich Supercomputing Centre

Supercomputer operation for

- Centre – FZJ,
- Regional – U. of Aachen
- Helmholtz & National – NIC, GCS
- Europe – PRACE, EU projects



Application support

- Traditional and SimLab support model
- Scientific visualization
- Peer review support and coordination

R&D work

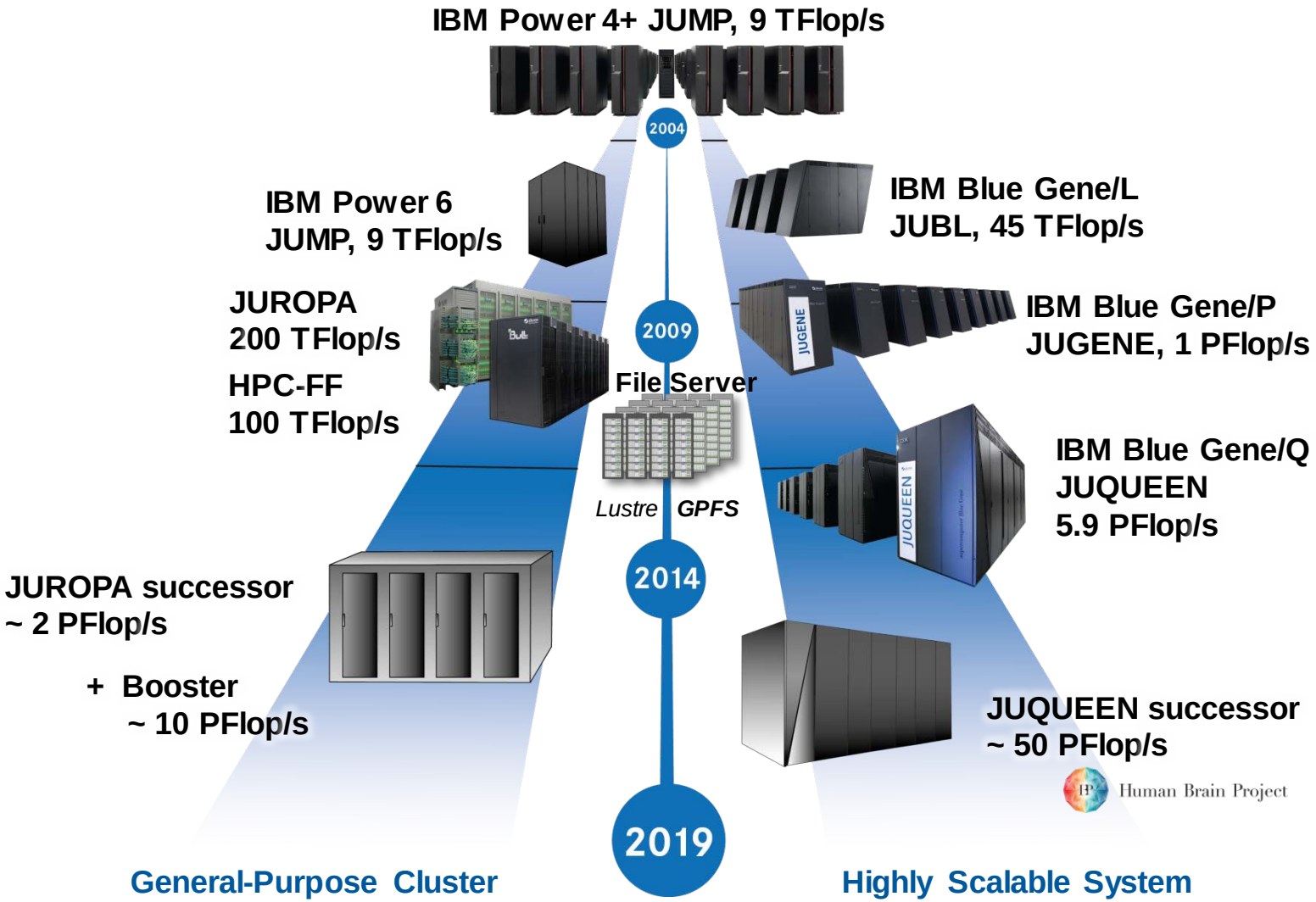
- Methods & algorithms, performance tools
- Community data management service
- Computer architectures (DEEP), Exascale Laboratories: EIC, ECL, NVIDIA

Education and Training

- Together with Aachen University of Appl. Sc. (BSc, MSc)
- GCS Prace Advanced Training Centre (PATC)
- CECAM node, International summer student programme

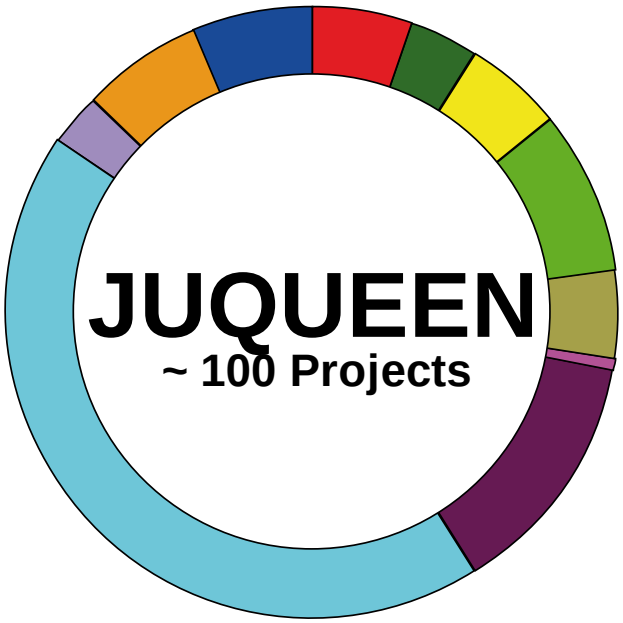
Head Count:
150 permanent
50 third party funded

HPC Systems: Dual Architecture Strategy



Research Fields of Current National Projects

Leadership-Class System

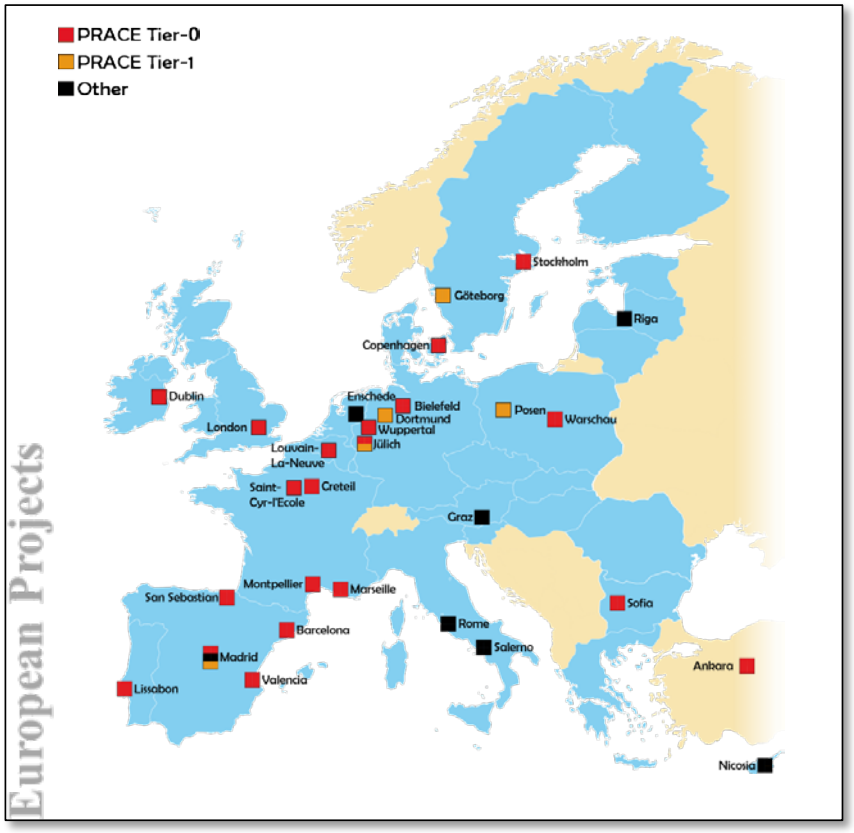


General-Purpose Supercomputer

Granting periods
05/2014 – 04/2015
11/2013 – 10/2014

- Astrophysics
- Biophysics
- Chemistry
- Earth & Environment
- Plasma Physics
- Soft Matter
- Fluid Dynamics
- Elementary Particle Physics
- Computer Science
- Condensed Matter
- Material Science

National and European Users @ JSC



Blueprint for Community-orientated Support

Staff

- Senior scientist recruited from scientific field
- 1-2 postdocs + technical staff (informatics)
- Jointly supervised PhD & MSc students

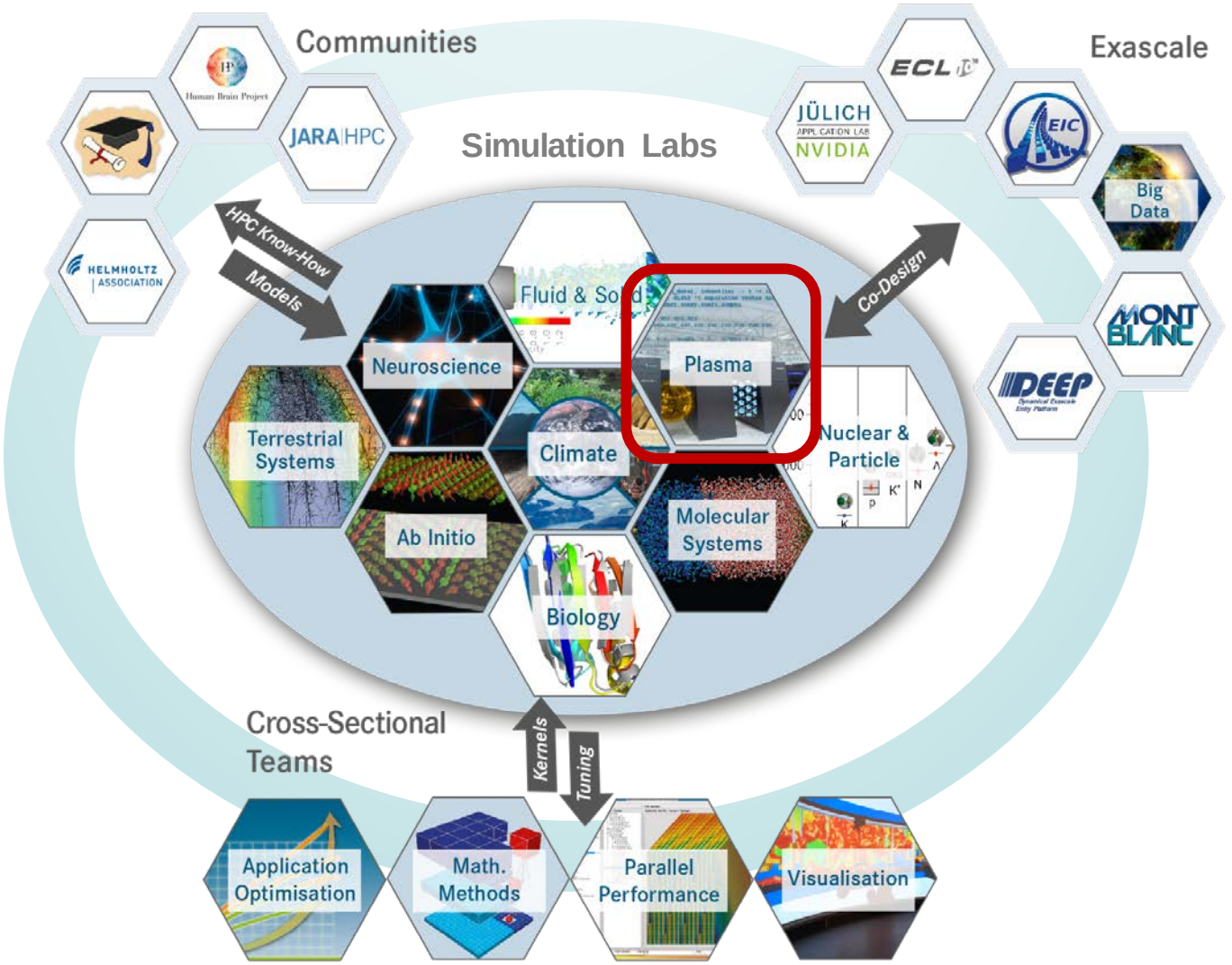
Support

- Porting/tuning/benchmarking
- Algorithm scaling
  Code clinic
- Workshops, schools

Research

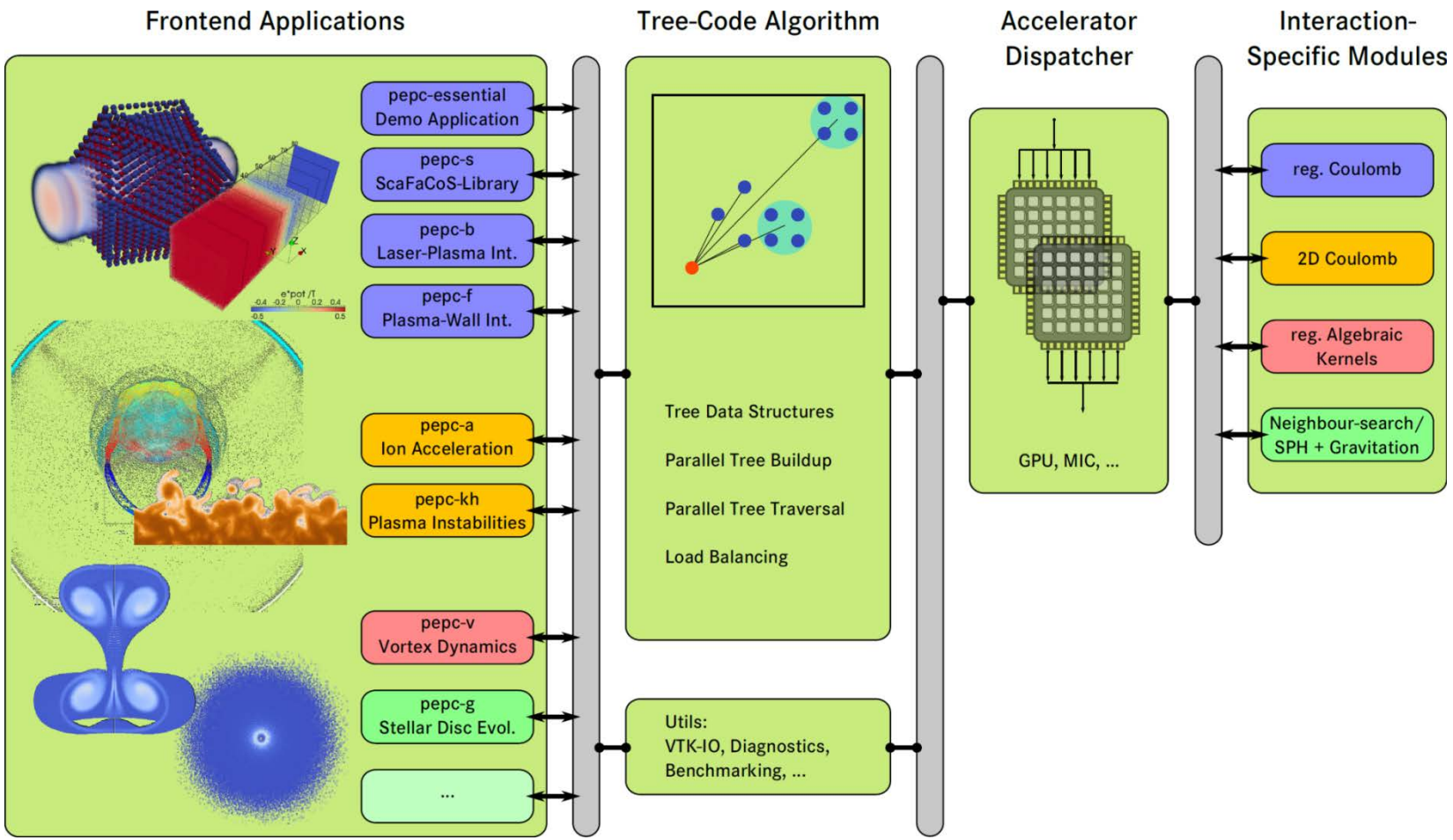
- Common/generic methods
- Scalable algorithms
- 3rd party projects

JSC Research & Support Environment

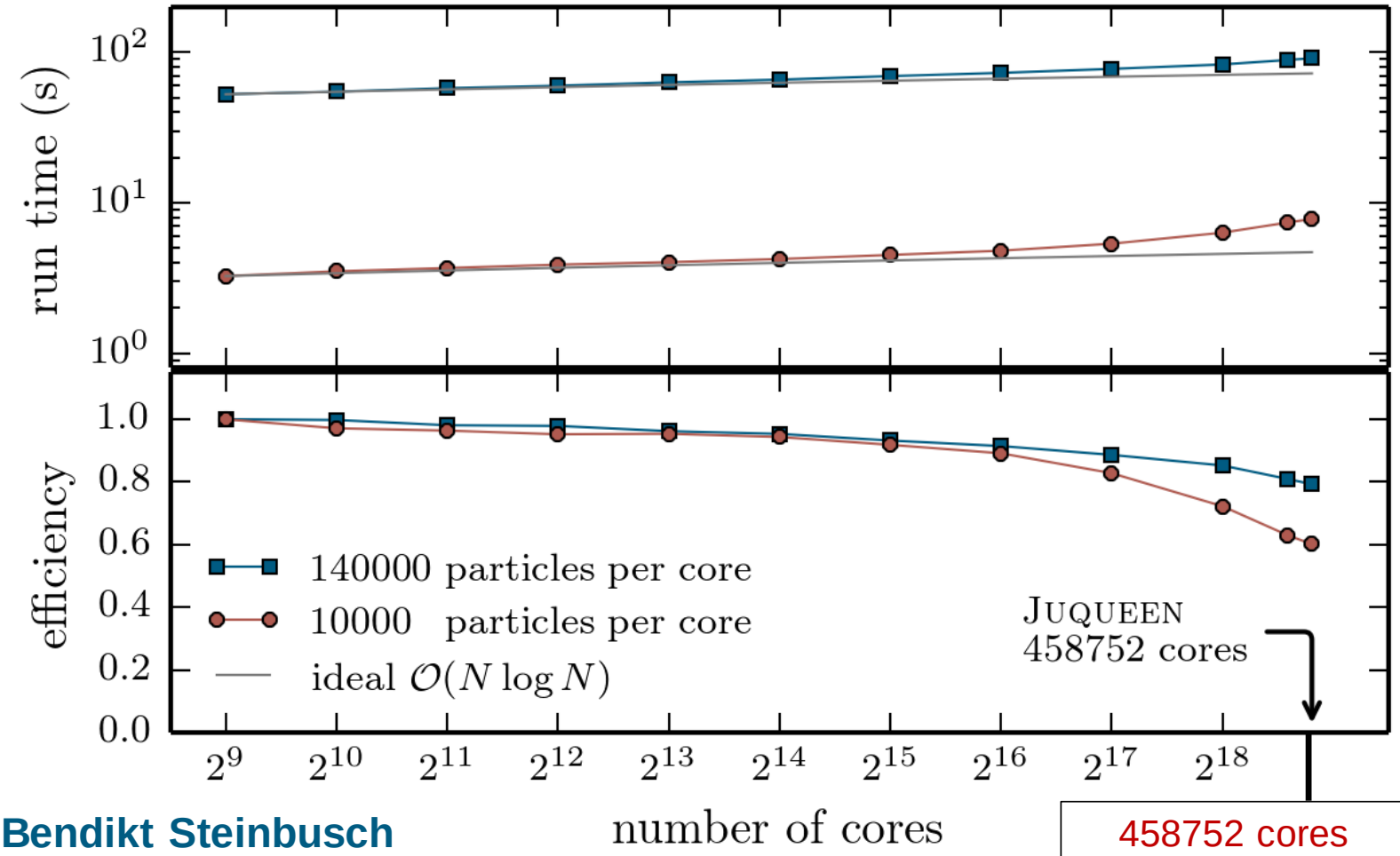


SimLab Plasma Physics: PEPC

PEPC - highly scalable, multi-physics tree-code framework



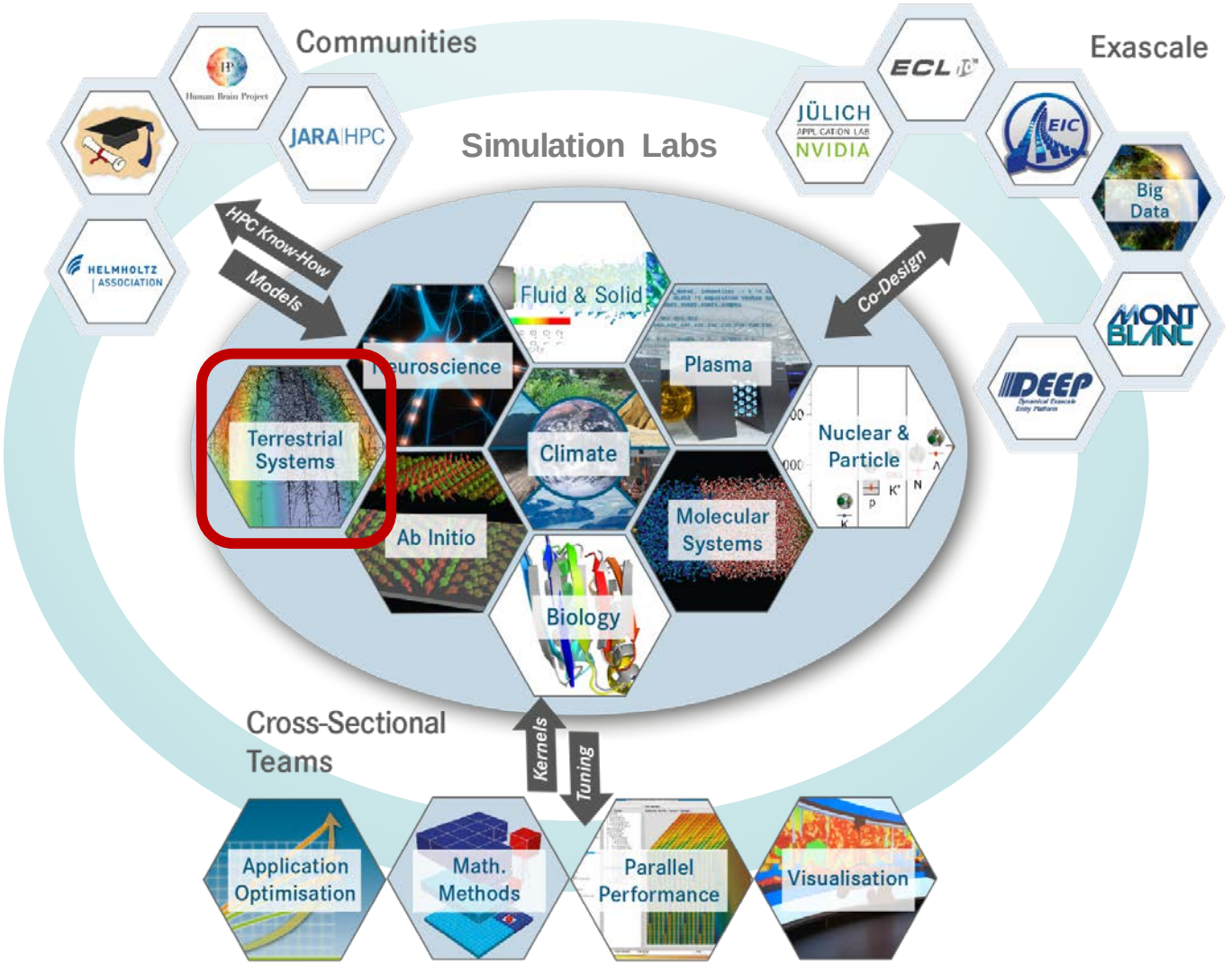
PEPC: Weak scaling on JUQUEEN



Bendikt Steinbusch (G8-NuFuSE)

458752 cores
1,668,196 parallel threads
64 x 10^9 particles

JSC Research & Support Environment



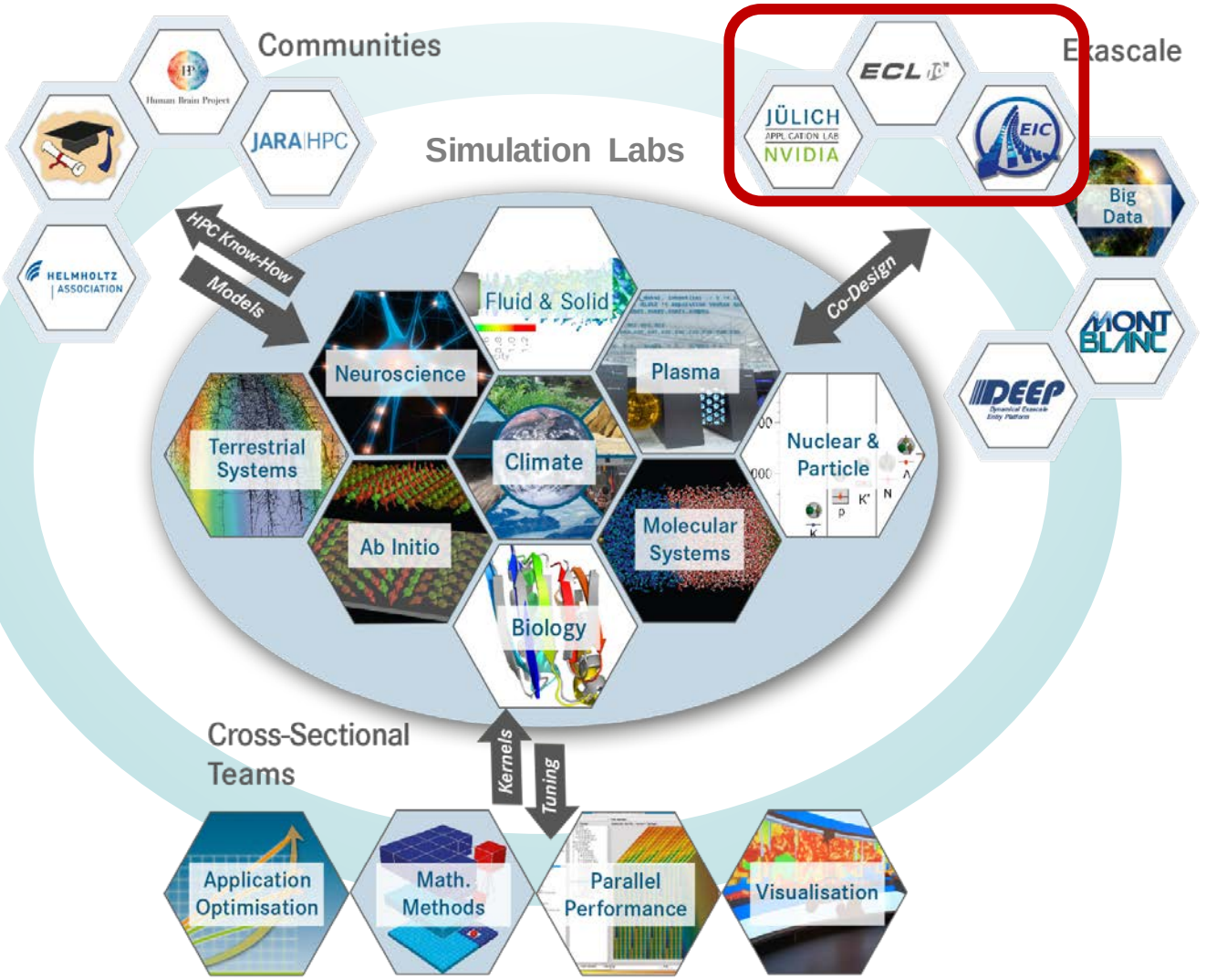
Simulation Lab *TerrSys*

TerrSysMP:

- Fully integrated groundwater-vegetation-atmosphere simulation platform; earth system models at regional scale
- Water cycle processes and variability across scales
- Climate and land use impacts

- Scalasca performance analysis
- Refactoring of OASIS-MCT coupling interface to remove scaling bottleneck
- Scaling now to 32k cores:
  64x increased problem size!

JSC Research & Support Environment



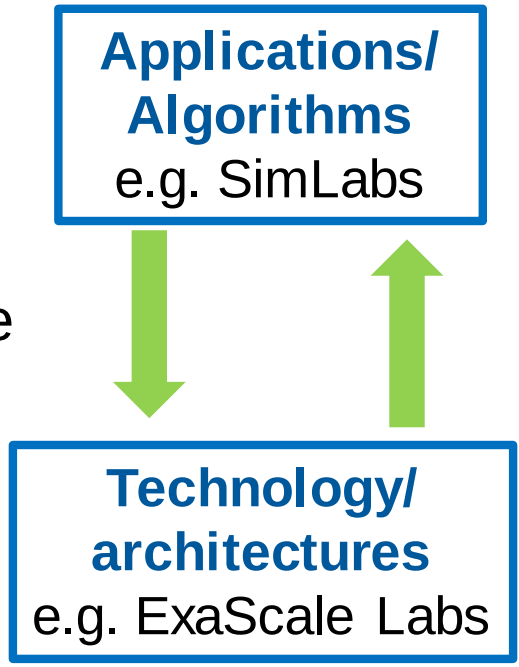
Exascale Research at JSC

Exascale challenges

- Drastically improve energy efficiency
- Preserve usability at tremendously increased level of parallelism
- Keep overall system balanced
- Address reliability and resilience

Co-design approach

- Scientific problem requirements influence architecture design and technology
- Architectural constraints impact formulation and design of algorithms and software



Co-design enabled through exascale labs

Exascale Research at JSC (cont.)

Established exascale labs

- Exascale Innovation Center (EIC) with IBM
  - Established in 2010
- ExaCluster Lab (ECL) with Intel and ParTeC
  - Established in 2010
- NVIDIA Application Lab at Jülich
  - Established in 2012

Topics addressed

- New architectural concept exploration
  - *Booster concept; Active storage architectures*
- Efficient and productive use of many-core architectures
- Richer memory hierarchies
- Scalability through new network technologies

Exascale Research at JSC: Examples of impact

DEEP: Enablement of new, high-performance network technology

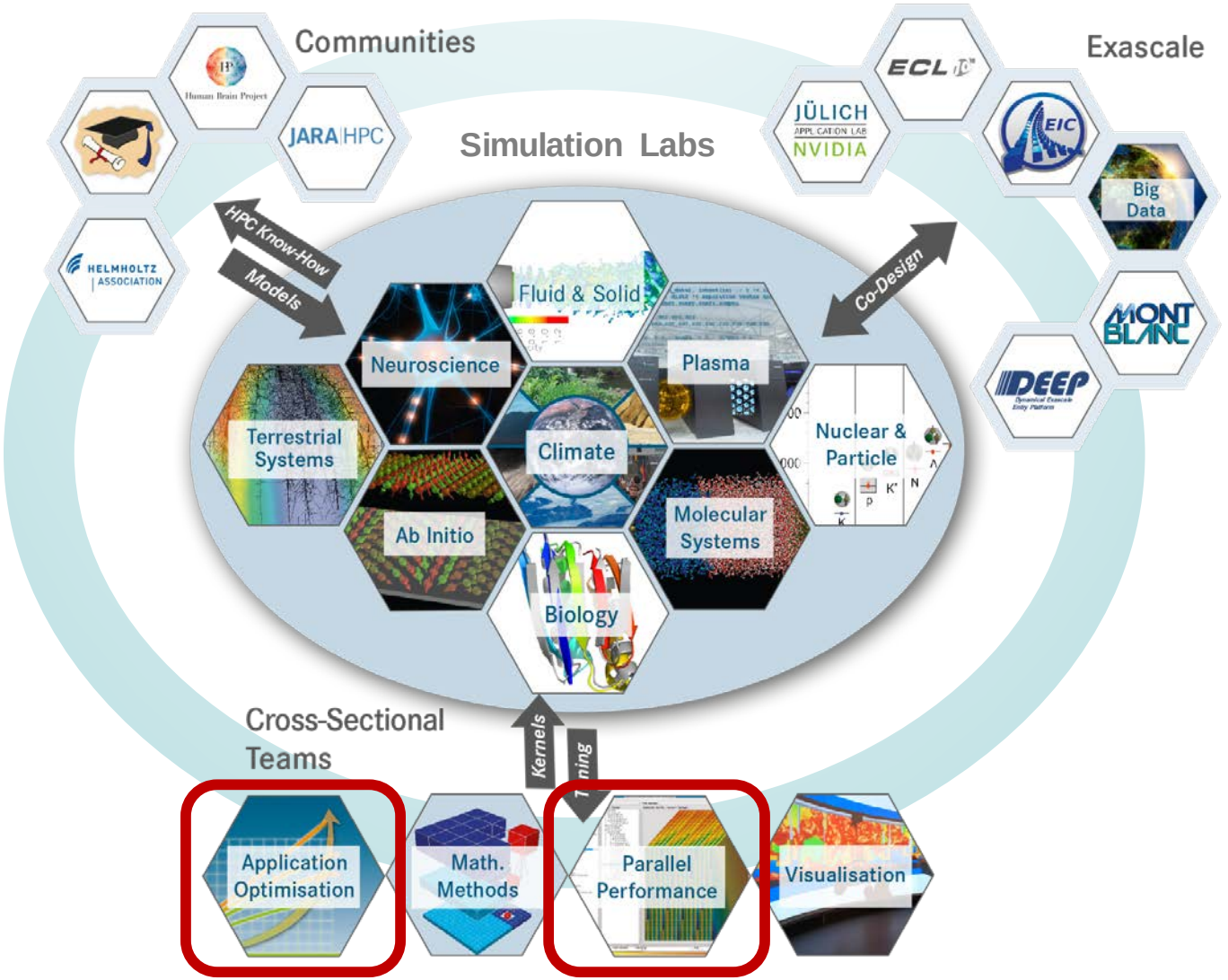
EIC: Design updates in the context of evaluation of concepts for memory for extreme systems

BGAS: Enablement of new active storage architectures

QPACE: Proof of energy efficiency (Green500)

JUROPA: Co-design of scalable cluster middleware and monitoring tools

JSC Research & Support Environment



Parallel Performance: Scalasca Overview

Scalable **A**nalysis of
Large **Sc**ale **A**pplications

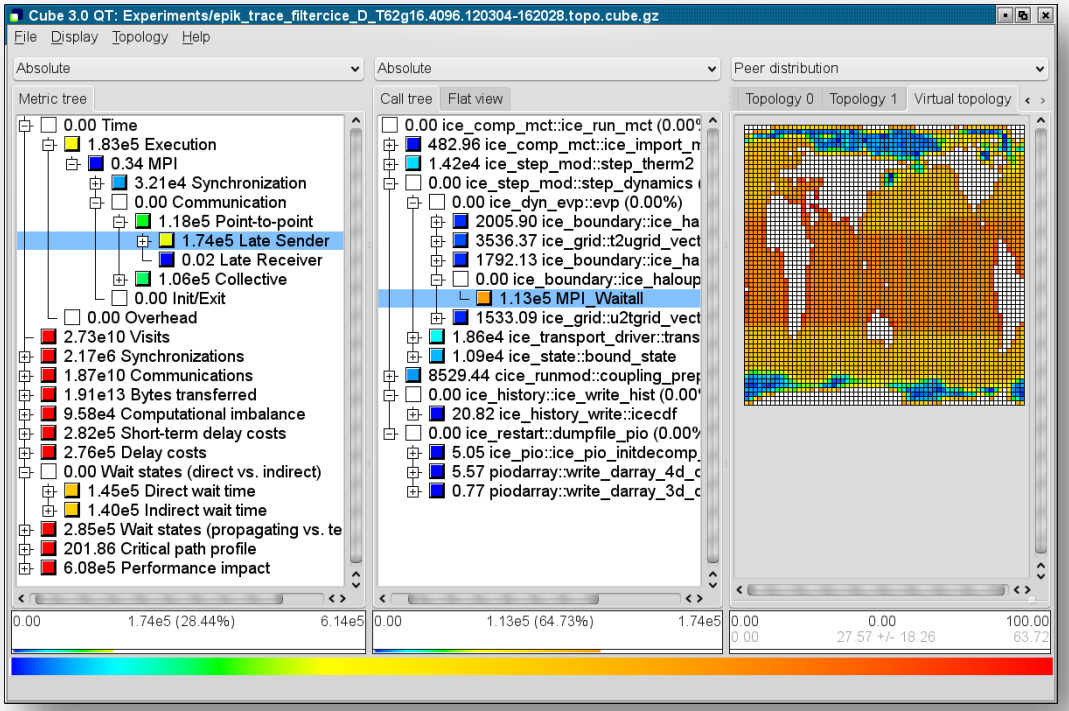
scalasca

http://www.scalasca.org/

Highly-scalable parallel performance tool

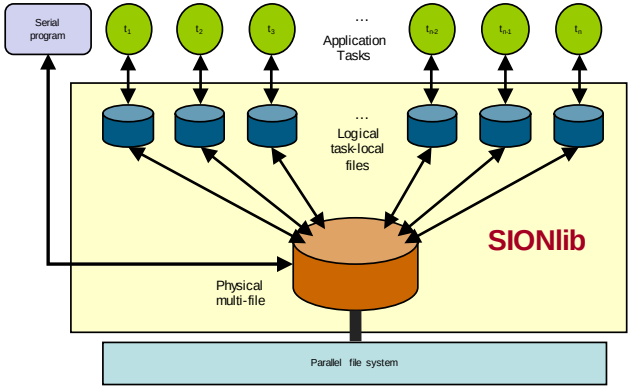
- Successful experiments with up to 1 million threads

Basis for user support, research and training

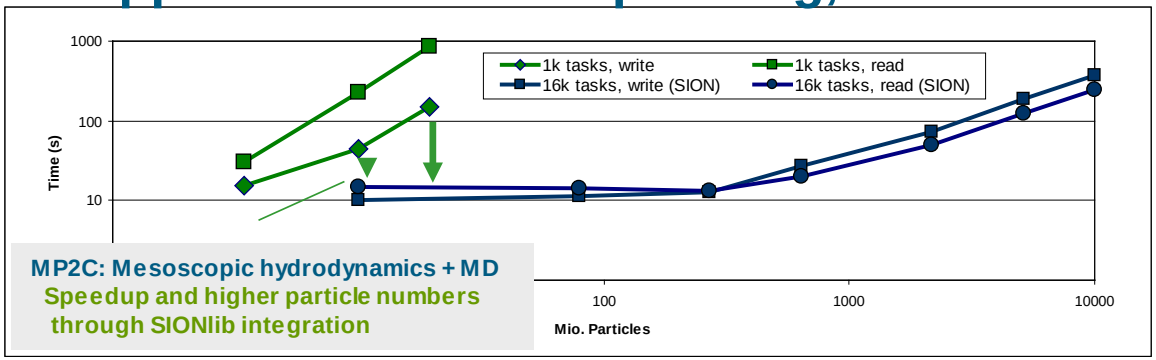


Application Optimization: SIONlib

SIONlib: Parallel I/O to task local files at large scale

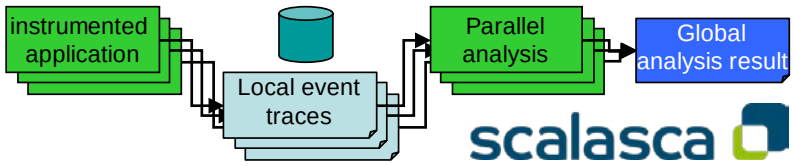


→ Applications: Check-pointing, Restart



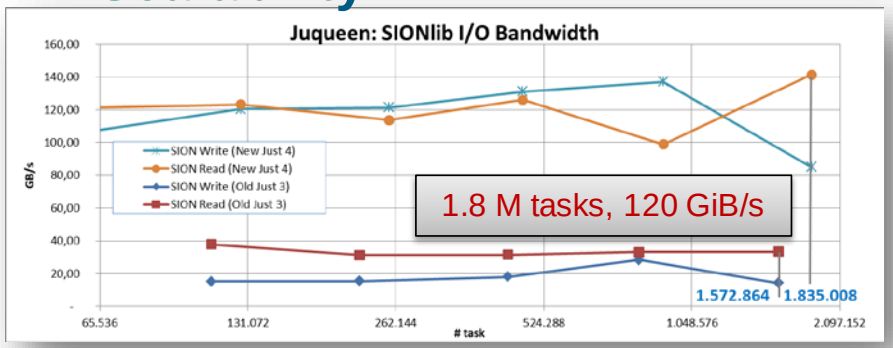
MP2C: Mesoscopic hydrodynamics + MD
Speedup and higher particle numbers through SIONlib integration

→ Tool Support



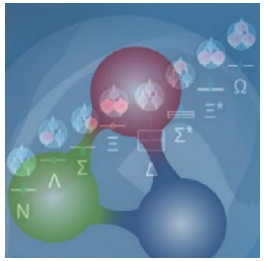
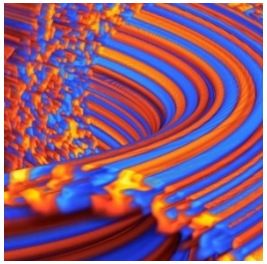
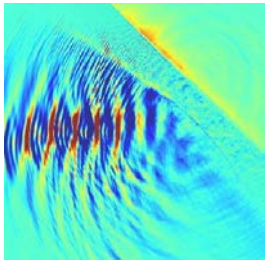
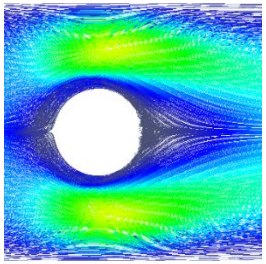
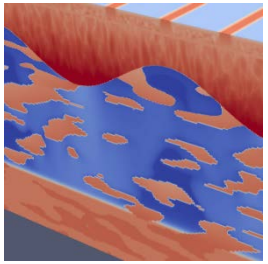
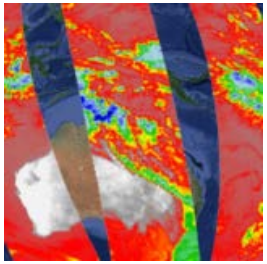
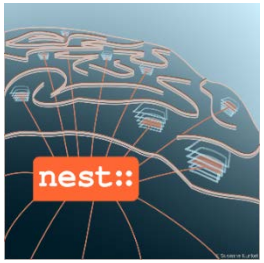
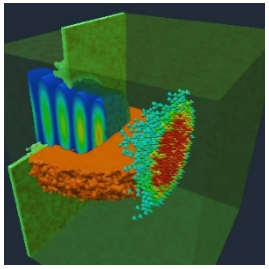
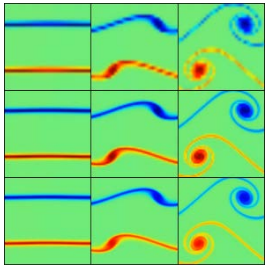
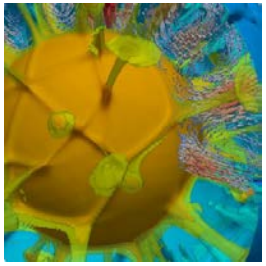
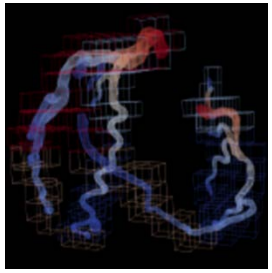
Score-P: Scalable Performance Measurement Infrastructure for Parallel Codes

→ Scalability



***JUQUEEN**: Total bandwidth (write/read) , one file per I/O-bridge (IOB) Just3 & Just4 GPFS file system*

High-Q Club: Exascale-Ready Applications on JUQUEEN

					
dynQCD	**GYSELA**	**JuSPIC**	**MP2C**	**muPhi**	**JURASSIC**
					
NEST	**PEPC**	**PMG+PFASST**	**TerraNeo**	**WaLBerla**	**OpenTBL**

12+ codes scaling across 458,752 JUQUEEN cores

WWW: http://www.fz-juelich.de/ias/jsc/EN/Expertise/High-Q-Club/_node.html

Potential Contributions to JLESC

- JSC is doing leading edge HPC technology development through Exascale Labs and its departments “HPC-Systems” and “Technology”

- JSC has established an internationally recognized expertise in domain-specific advanced application support through its SimLabs and its Cross-Sectional Teams